Office of Science / Basic Energy Sciences (BES) Program at LLNL

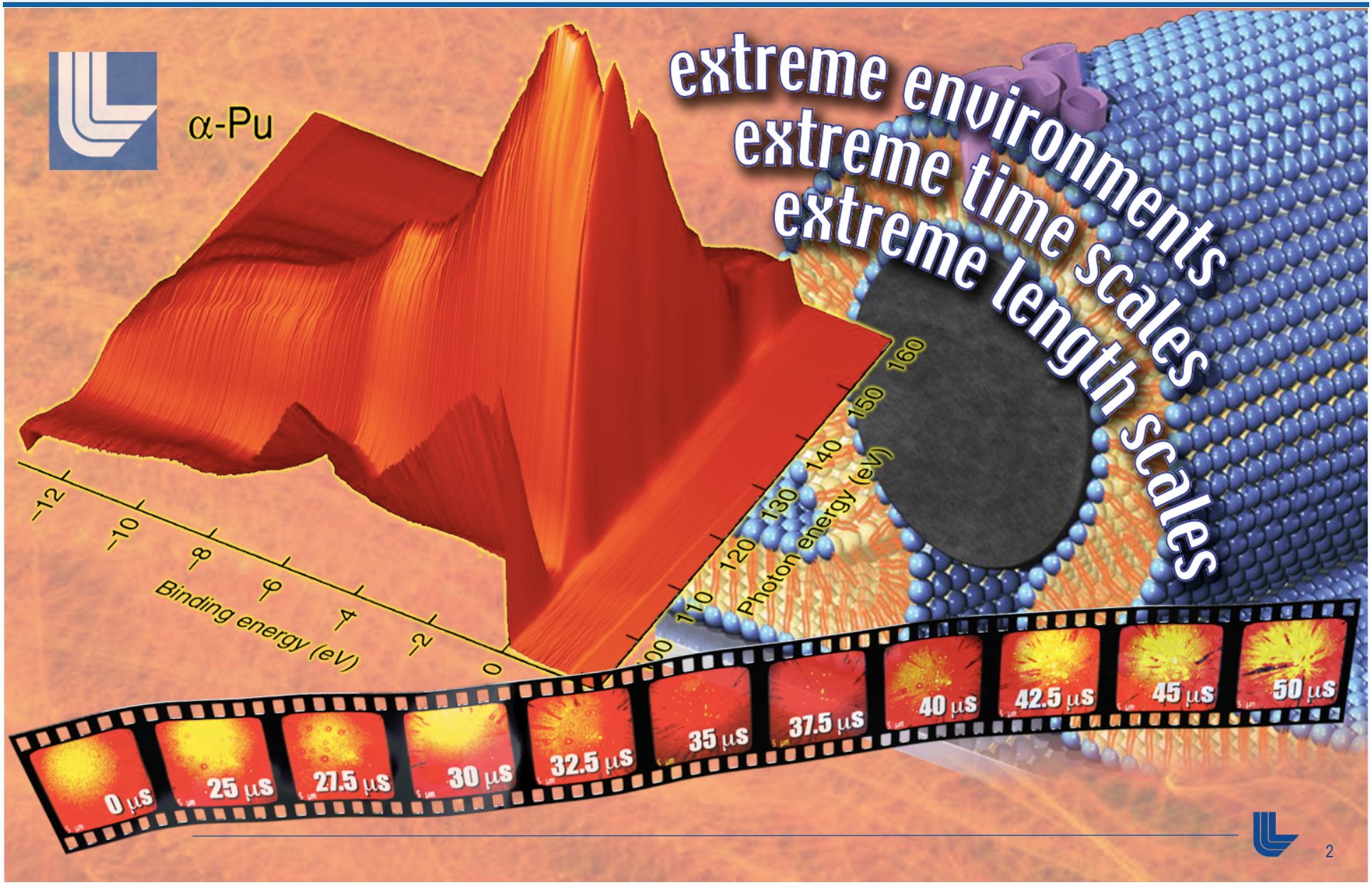
January 24, 2011

Christian Mailhiot
BES Laboratory Coordinator
Lawrence Livermore National Laboratory

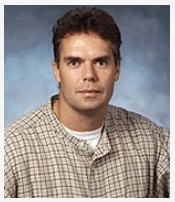
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

LLNL-PRES-465876-DRAFT

Time- and length scale-resolved investigations of materials in extreme environments underpin the BES program at LLNL



LLNL portfolio: BES/Materials Sciences and Engineering Division

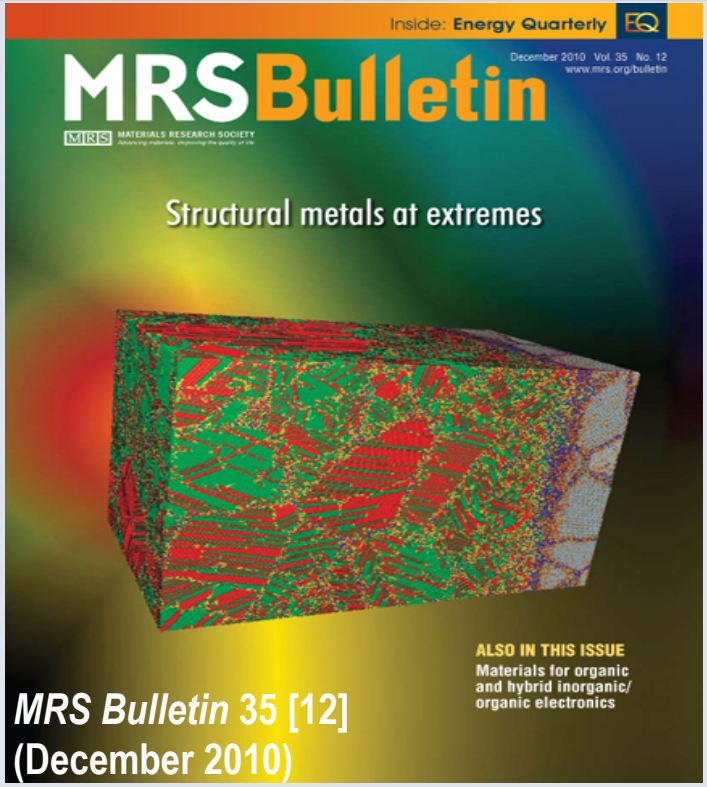
BES/DMS&E-funded project	Principal investigator
Fundamental Mechanisms of Transient States in Materials Quantified by Dynamic Transmission Electron Microscopy (DTEM)	 Geoff Campbell  Nigel Browning
Investigations of electron correlation in complex systems	 Jim Tobin
Virus assembly at nanoscale chemical templates	 Tony van Buuren
Evolution of Grain Boundary Networks in Extreme Radiation Environments (SISGR)	 Mukul Kumar

LLNL portfolio: BES/ChemGeoBiosciences

BES/ChemGeoBiosciences-funded project	Principal investigator
Geophysical electric resistance tomography in porous media	Charles Carrigan
Mineral precipitation kinetics using NMR spectroscopy	 Susan Carroll
Geochemical imaging with nano-SIMS II	 Rick Ryerson
Kinetic isotope fractionation	 Ian Hutcheon

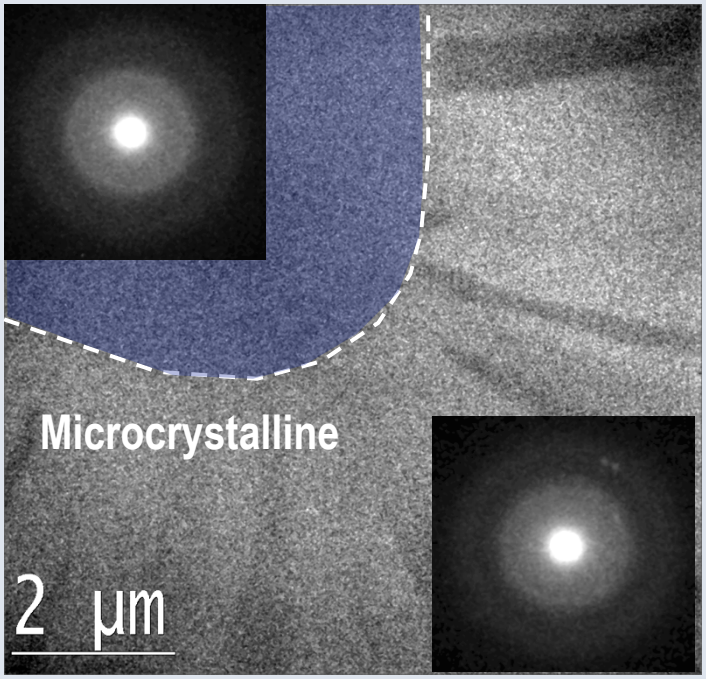
The BES-supported DTEM project enables high-impact science and enhances LLNL's programs in materials under extreme thermomechanical environments

New capabilities for high-impact science



"In situ characterization of metals at extremes" by N.D. Browning, G.H. Campbell, J.A. Hawreliak, and M.A. Kirk" [*MRS Bulletin* 35 [12] 1009 – 1016 (December 2010)]

Kinetics of phase transformations



- Single-shot, 15 ns time-resolved images and diffraction patterns reveal the rapid solidification process after pulsed laser melting of Al
- Morphological changes in liquid-solid interface of rapid lateral solidification of molten Al and quantitatively measured interface velocities

PI: Campbell

The dynamic transmission electron microscopy (DTEM) project has received several awards from the scientific community

2008-Dynamic Transmission Electron Microscope, which provides the highest resolution ever for digital imaging of ultrafast material processes on the billionth of a meter scale.

2010-Microscopy Today's MT-10 Awards recognize the best new products and methods across the entire field of microscopy. Five of the awards are primarily related to the life sciences and five are related to the physical sciences.

2008-Nano 50 recognizes the top 50 technologies, products and innovators that have significantly impacted, or are expected to impact, the state of the art in nanotechnology.

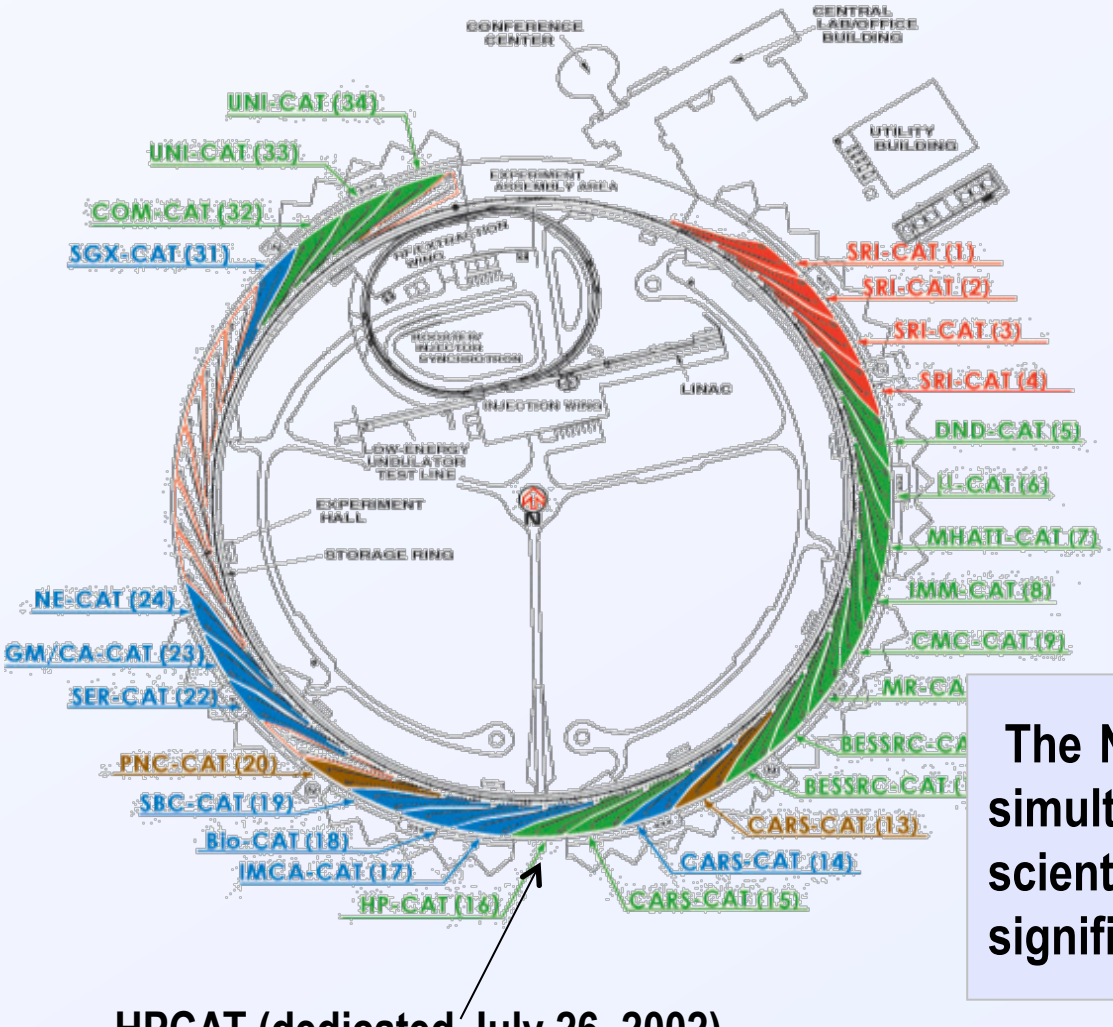
The DTEM at LLNL (Bldg. 235)

- Capability to characterize transient events in materials far from equilibrium and under different environmental conditions
- Makes LLNL a pioneer for real-time, *in situ* investigations of materials dynamics with unprecedented temporal and spatial resolution

PI: Campbell, Browning, LaGrange, Reed, King

The High-Pressure Collaborative Access Team (HPCAT) at the APS has been a very successful and scientifically productive NNSA-BES-academic partnership to advance the field of compression science

Advanced Photon Source (APS)



HPCAT (dedicated July 26, 2002)

- Four beamlines: 2ID, 2BM
- Nine hard x-ray hutches
- HP-CAT partners: BES (30 %); NNSA (30 %), CIW (30%), LLNL (10 %)

The NNSA-BES-CIW HPCAT partnership simultaneously and uniquely enables scientific discoveries and contributes to significant LLNL mission deliverables.

The BES-supported research in strongly-correlated materials provides scientific underpinnings to LLNL's programs in actinide science and technology for national security and energy applications

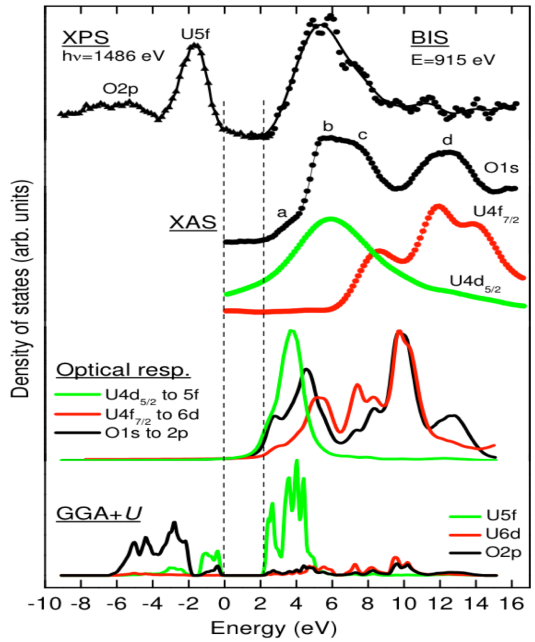
Complexity and emergent phenomena

MRS Bulletin 35 [11] (November 2010)

- Kevin T. Moore, LLNL – Guest Editor
- (*) S.-W. Yu *et al.*, *"A demonstration that UO_2 is an f-f type Mott-Hubbard insulator,"* in preparation.

Actinide science and technology

UO_2



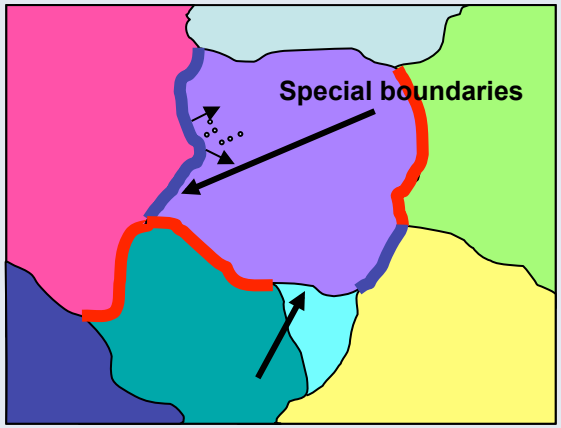
- UO_2 is a widely used nuclear fuel and exhibits strong electron correlation effects (*)
- Investigations of UO_2 with spectroscopic techniques:
  - X-ray absorption (XAS),
  - X-ray emission (XES),
  - Bremstrahlung Isochromat Spectroscopy (BIS),
  - Resonant Inverse Photoelectron Spectroscopy (RIPES)
  - Photoelectron Spectroscopy,

PI: Tobin

BES-supported fundamental research on radiation-tolerant materials enhance LLNL's programs in materials development for advanced nuclear energy systems

Grain boundaries in irradiated materials

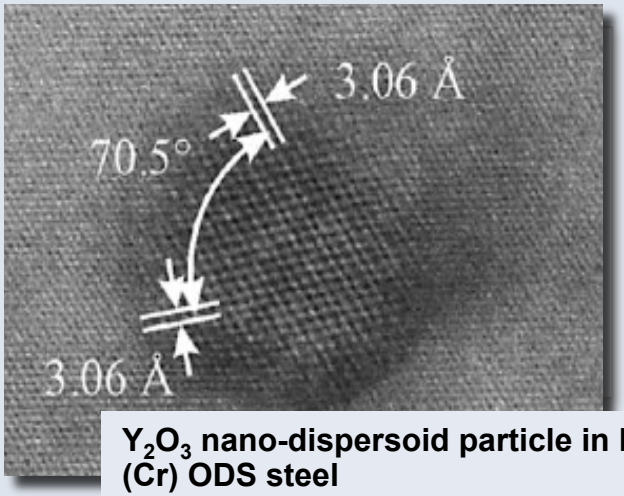
- High grain-boundary densities can retard radiation damage, but the microstructure will tend to be unstable in the long term
- Potential changes to boundary crystallography and morphology as the free energy increases with defect absorption under irradiation are poorly understood



Interfaces with high degree of disordering (high free volume) are good zero-bias point defect sinks

Special boundaries pin the random boundaries at triple junctions leading to a retardation in grain coarsening

Materials development for advanced nuclear energy systems



Y_2O_3 nano-dispersoid particle in Fe (Cr) ODS steel

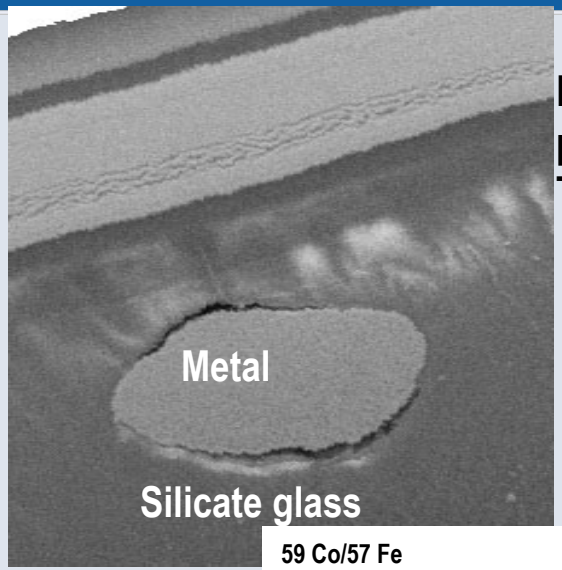
- Manipulation of structures over a broad range of length scale
- Testing and characterization:
  - Ion beam irradiation
  - TEM
  - Mechanical testing
  - Small-scale characterization

PI: Kumar, Belak, Bernier, Bulatov, Lagrange, Reed, Tang (Lawrence Fellow)

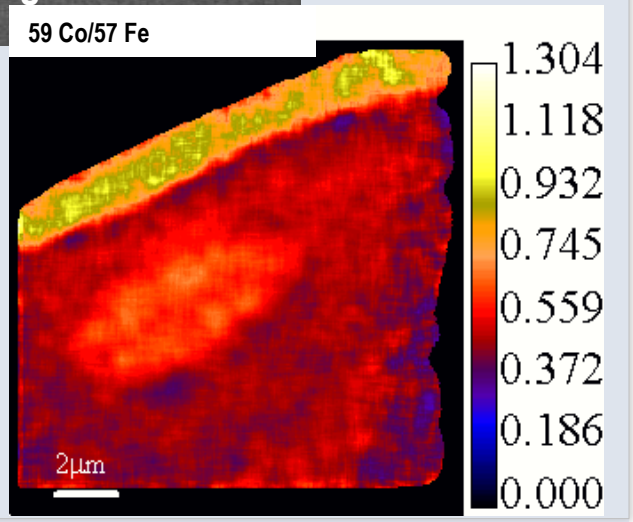
BES-funded projects apply unique materials characterization capabilities to problems in geophysics and geochemistry

- BES project (Ryerson, Weber) focuses on trace element analysis of materials synthesized under extreme conditions of pressure and temperature
- Synergy and "dual-use" with LLNL nuclear forensic projects.

Geochemical imaging with NanoSIMS



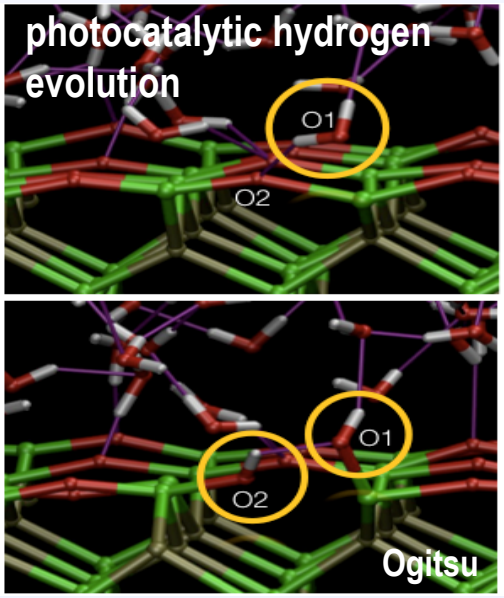
Laser-heated DAC
p = 60 GPa
T = 4000 K



PI: Ryerson, Weber, Carroll, Carrigan

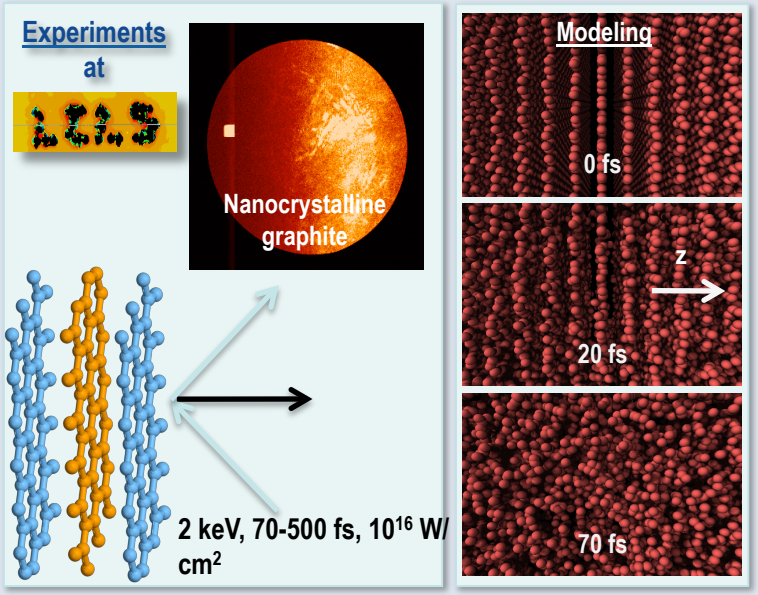
We are putting forward future initiatives in computation materials science chemistry for energy applications and ultrafast x-ray science

Computational chemistry for energy applications



- Quantum Monte Carlo simulation of many-body systems
- Discovery of novel materials by quantum simulations
- Fundamental mechanisms of energy conversion
- Theoretical and computation chemistry
- Finite-T quantum simulations of lattice dynamics
- Dislocation dynamics and μ-structure evolution

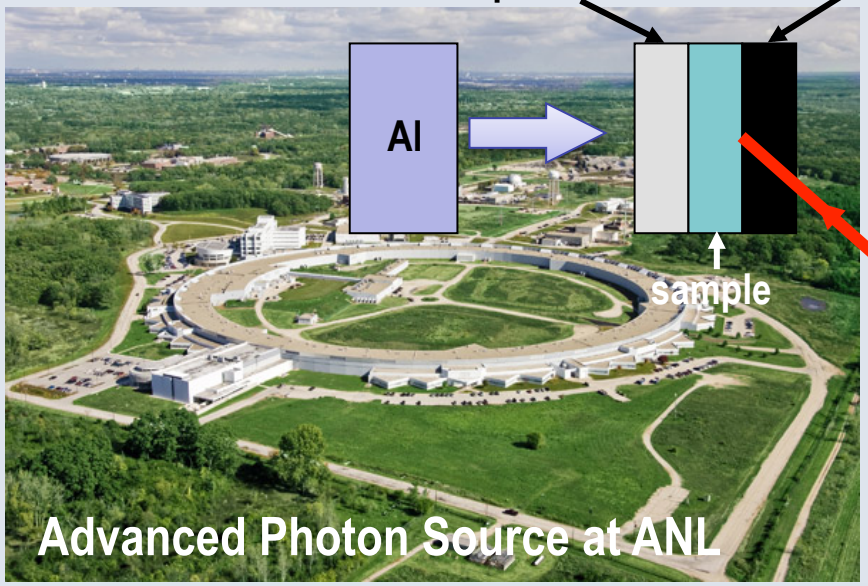
LCLS ultrafast x-ray for dynamic compression science

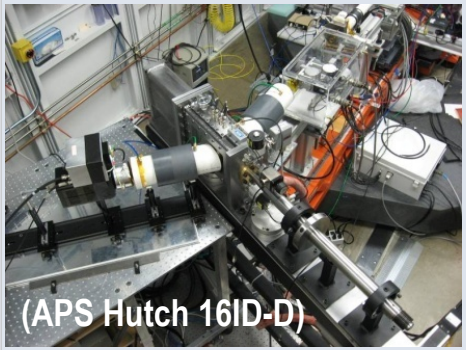


- Ultrafast nanoscale dynamic imaging using x-ray free electron lasers
- Coherence-preserving x-ray adaptive optics

A proposal has been put forward for a NNSA-BES partnership to establish a dynamic compression capability at the Advanced Photon Source (APS)

Dynamic Compression Collaborative Access Team (DC-CAT)

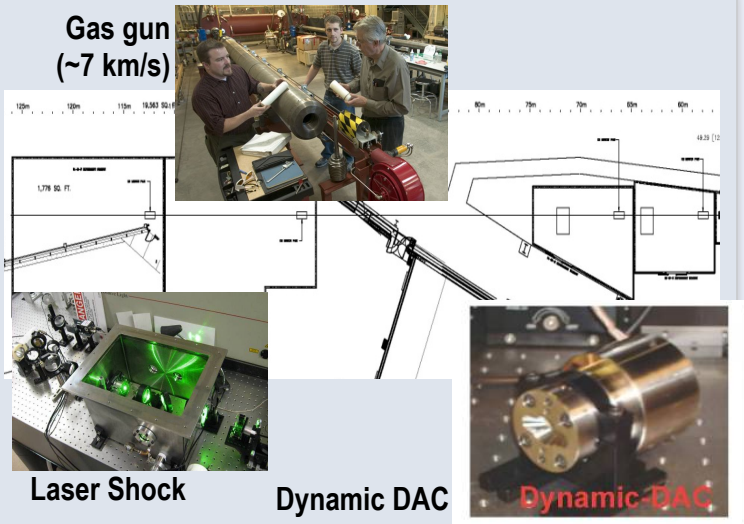




Small powder guns (~1.5 km/s)

- Proof-of-principles shock compression experiments on LiF, Al, and Cu have been performed at the HP-CAT facility at the APS
- Jensen and Gupta, *Journal of Applied Physics*, 104(1): 013510 (2008).

DC-CAT design



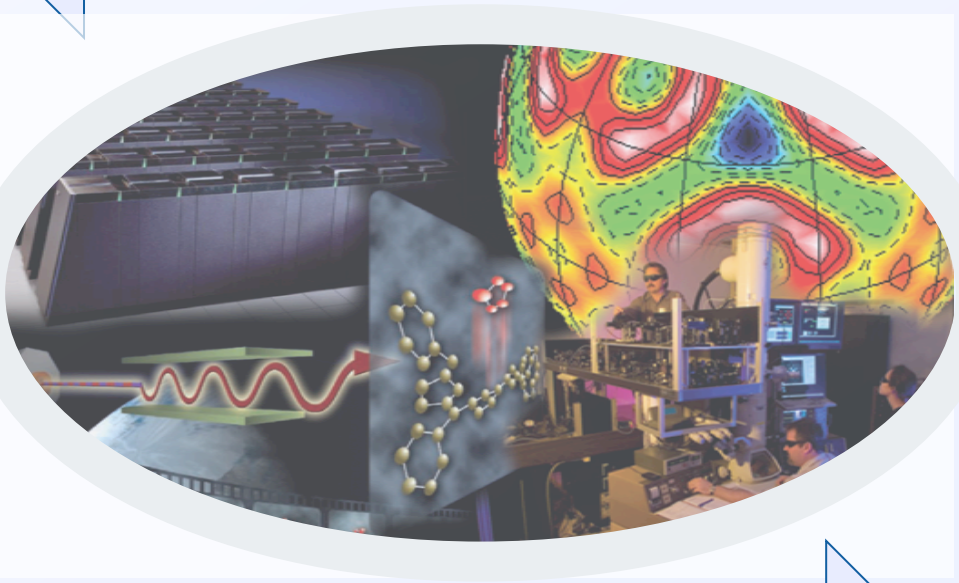
- Multi-institution proposal (WSU lead)
- Capability for time-resolved investigation of dynamic response in condensed matter
- Integrates dynamic drivers and x-ray capabilities
- Proposal for a 2-phase approach submitted to NNSA in December 2010
- Briefed to BES in February 2010

The LLNL-BES partnerships provide an important foundation that enhances fundamental science for program execution and development

LLNL

- Actinide science and technology
- Materials in extreme environments
- Materials development for advanced nuclear energy systems
- Geosciences

Capabilities and workforce contributing to mission-supporting programs



Mission-derived challenges leading to scientific breakthroughs

BES

- Complex and emergent behavior in condensed matter
- Master the control of energy-relevant complex systems
- Manage radiation effects in materials
- Physical and chemical understanding of geological processes

BES investments at LLNL have significant strategic impact and LLNL values its sustained partnership with BES